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Expander Graphs and Low-Distortion Embeddings for Learning on Graphs

Graphs are a natural model for many domains we would like to learn on, and graph neural networks based on local message passing have seen success on various problems. In other areas of machine learning, however, Transformers (based on pairwise "attention") are the dominant recent machine learning model. Yet Graph Transformers have had significant scaling problems because of the quadratic full everything-to-everything attention. This talk presents a line of work addressing this problem: first, in Exphormer ("expander" + "transformer"), we exploit expander graphs to create a sparse graph to augment the original problem graph, for limited attention but good expansion properties across layers. Exphormer helps scale (computationally and statistically) graph Transformers to much larger graphs, obtaining state-of-the-art results on many kinds of graph problems. On many very large graphs (e.g. social networks or protein-protein interaction networks), though, even the original problem's graph is too large for practical learning; we thus build an extension called Spexphormer ("sparse Exphormer"), which further constrains attention to "important" edges, dramatically reducing memory usage. We finally present a theoretical account of situations where Spexphormer's sparsification is possible, and where it is not.